STUDIES ON THE QUASI-POTENTIAL METHOD FOR THE INVERSION PROBLEM IN ION-ATOM ELASTIC SCATTERING

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Using the quasi-potential form of the phase shifts in the JWKB approximation and choosing a particular functional form to insure the correct behaviour of the ion-atom interaction we have constructed the potential through the Sabatier transformation. Numerical computations are given for the ion-atom case.

1. Introduction

The experimental physicist is often interested in deducing the scattering potential $V(r)$, directly from his measurements rather than predicting the cross section for assumed forms of the potential. For this inversion problem there exist, in general, three kinds of formalisms which can be summarized as follows:

In the first [1–5], using physical considerations, it is assumed that the JWKB approximation is valid for the phase shifts and since the Sabatier transformation under special assumptions is bijective, we can define a quasi-potential from which $V(r)$ can be derived. The phase-function is simulated by a several-parameter formula which enables us to use the Weyl-transform,

$$\tilde{\xi}(\beta) = \int_{\beta}^{\infty} d\tau\tau\xi(\tau)/\sqrt{\tau^2-\beta^2} = \int_{0}^{\infty} ds\xi\{\sqrt{\beta^2+s^2}\}$$

for the inversion problem.

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The second [6] gives a positive answer to the inversion problem for special sets of phase shifts and potentials of the Yukawa class.

The third approach [7] can be considered as an extension to the inversion problem of the Gel'fand Levitan formalism.

Because the first formalism is derived in a way that the numerical computations are feasible, we use it for the case of elastic collisions between ions and noble gases.

In Section 2 we briefly describe the quasi-potential form of the phase shifts. In Section 3 numerical procedures and results are shown.

2. *Quasi-potential formalism*

In this Section we review briefly the quasipotential formalism. It will be suitable to use the standard dimensionless abbreviations

$$x = \frac{r}{r_m}, \quad A = kr_m, \quad K = \frac{E}{\varepsilon} = \frac{A^2}{B},$$

$$P(x) = \frac{V(r)}{\varepsilon}, \quad B = \left(\frac{2\mu}{t^2}\right) r_m^2 \varepsilon, \quad \beta = (l+\tfrac{1}{2})/A, \tag{1}$$

where r_m is the value of r at the minimum of the potential $V(r)$, ε—the depth of the minimum, μ—the reduced mass, $E = \hbar^2 k^2/(2\mu)$ — the kinetic relative energy, and l—the angular momentum. Using the Sabatier transformation [8]

$$t = x\left(1 - \frac{P(x)}{K}\right)^{1/2}, \tag{2}$$

its inversion $x = x(t, K)$, and defining the energy-dependent quasi-potential

$$Q(t, K) = 2K \ln\left[\frac{x(t, K)}{t}\right] = -K \ln\left[1 - \frac{P(x(t, K))}{K}\right], \tag{3}$$

we can write the well known JWKB-formula for the phase shifts δ_l^{JWKB} as $\delta_l^{\text{JWKB}} = A\eta(\beta, K)$

$$\eta(\beta, K) = -\frac{1}{2K} \int_{\beta}^{\infty} dt t Q(t, K)/(t^2 - \beta^2)^{1/2}. \tag{4}$$

The problem of constructing an equivalent potential for a given set of phase shifts $\eta(\beta, K)$ is solved if we consider Eq. (4) as an integral equation. This can be then solved to give the quasi-potential

$$Q(t, K) = \frac{2K}{\pi} \int_{\tau}^{\infty} d\beta \theta(\beta, K)/(\beta^2 - \tau^2)^{1/2}, \tag{5}$$

where $\theta(\beta, K) = 2\dfrac{\partial}{\partial\beta}\eta(\beta, K)$ and β is consider now as a continuous variable.

For a given K, the value of x corresponding to t is obtained by writing the relation (3) as

$$x(t, K) = te^{Q(t,K)/(2K)}. \tag{6}$$

Using Eq. (6), it is easy to construct the potential $P(x)$, because according to Eq. (3)

$$P(x) = K(1-e^{-Q(t,K)/K}). \tag{7}$$

The conditions under which this inversion procedure works are the following:
(a) $V(r) \leqslant E$, or $P(x) \leqslant K$, otherwise $t(x, K)$ would be a complex function.
(b) The mapping $x \leftrightarrow t$, defined by Eq. (2), must be bijective, otherwise the inverse function $x = x(t, K)$ is not unique. Of course, there is a critical value of K, say $K = K_0$, which puts

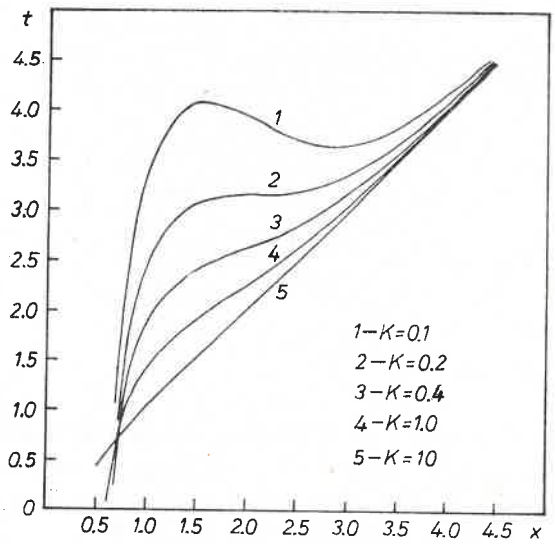

Fig. 1. The mapping defined by Eq. (2) for different values of K taking a modified Morse potential

a lower limit to the application of the theory. In fact, the monotonous behaviour of $t = t(x, K)$, K a parameter, exists for $K > K_0$ and ceases for $K < K_0$. This is shown in Fig. 1 where we have plotted t vs. x for different values of K taking a modified Morse potential [9]; it can be seen that $K_0 = 0.2$.

3. Application to the ion-atom case

The potential of interaction between an ion and an atom shows a strong repulsion at small distances, a minimum at equilibrium distance, and behaves according to the form $P(x) = -a/x^4$ at large distances. The phase function $\eta(\beta, K)$ also has a typical behaviour which can be simulated by an empirical function containing a small number of parameters which may be evaluated by fitting the theoretical cross sections to results of experimental

measurements. In this work we use the following ten-parameter formula for the phase-function:

$$\eta(\beta, K) = \frac{1}{2K}[f_1+f_2+f_3],$$

$$f_1 = \frac{\pi}{2}(a\beta-b)e^{-\gamma\beta},$$

$$f_2 = \frac{\sqrt{\pi}}{2}\left[\frac{C_1}{r_1}e^{-\gamma_1{}^2\beta^2} - \frac{C_2}{r_2}e^{-\gamma_2{}^2\beta^2}\right],$$

$$f_3 = d\left(\frac{1}{(d_1+\beta^2)^{1/2}} - \frac{1}{(d_2^2+\beta^2)^{1/2}}\right). \tag{8}$$

The "deflection function" $\theta(\beta, K)$ may be evaluated. Then, we use the Weyl transform and obtain from Eq. (5) an explicit form for the quasi-potential

$$Q(t, K) = Q_0+Q_1+Q_3,$$

$$Q_0 = (a+\gamma b)K_0(\gamma t)-a\gamma tK_1(\gamma t),$$

$$Q_1 = -(C_1e^{-\gamma_1{}^2t^2}-C_2e^{-\gamma_2{}^2t^2}),$$

$$Q_3 = d\left(\frac{1}{d_1+t^2} - \frac{1}{d_2+t^2}\right), \tag{9}$$

where $K_0(y)$ and $K_1(y)$ are modified Bessel functions of the second kind [10]. Of course, the quasi-potential $Q(t, K)$ has by fixed K the same typical behaviour as the interaction potential: Q_0 sketches the strong "repulsion" at small t, Q_1 represents a potential well, where the parameters define the form and deepness of the well, and Q_3 determine the behaviour for large t. Expansion shows that

$$Q_3 = \frac{d(d_2-d_1)}{t^4} + \frac{d(d_1^2-d_2^2)}{t^6} + \frac{d(d_2^3-d_1^3)}{t^8} + \ldots,$$

which corresponds to the polarization and higher multipole interactions.

From Eq. (3) it is seen that the quasi-potential $Q(t, K)$ depends on K at difference in the potential of $P(x)$. This means that the parameters γ, a, b, c_1, γ_1, c_2, γ_2, d, d_1, d_2 also depend on the energy. To obtain information about this energy dependence, we have proceeded as follows:

(a) Using Eqs. (3) and (4), we have calculated for different energies the set of phase shifts $\eta(\beta, K)$ as a function of β for a known potential $P(x)$ [9].

(b) For each K we have then evaluated the parameters by fitting the theoretical $\eta(\beta, K)$ to the ten-parameter formula Eq. (8). The results are shown in Table I.

Figs. 2–6 show the influence of the parameters on the resulting quasi-potential. A suitable choice of parameters allows us to shift the minimum, to influence the curvature,

TABLE I

Energy dependence of the parameters in Eq. (8)*

	10 eV	9 eV	7 eV	5 eV	4 eV
γ	5.5	5.5	5.0	5.0	4.99
a	5.7	7.0	7.6	8.0	8.4
b	5.7	5.0	4.5	3.8	3.0
c_1	2.2	2.2	2.2	2.2	2.2
γ_1	0.73	0.71	0.70	0.68	0.68
c_2	3.6	3.6	3.6	3.65	3.68
γ_2	1.41	1.40	1.35	1.30	1.27

* The parameters d, d_1, d_2 are omitted since the present example is not very sensitive to these parameters.

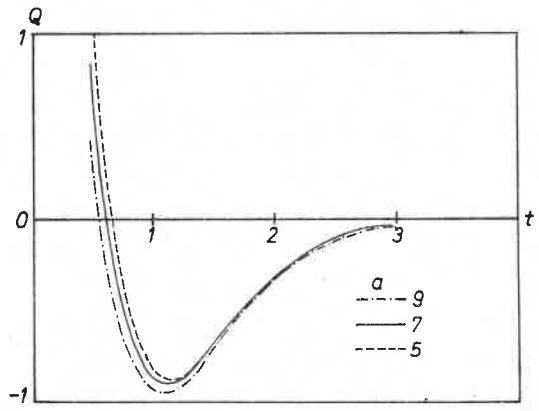

Fig. 2. The influence of parameter a on the quasi-potential

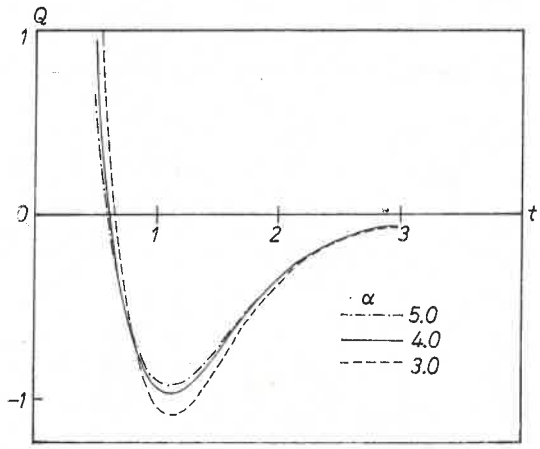

Fig. 3. The influence of parameter α on the quasi-potential

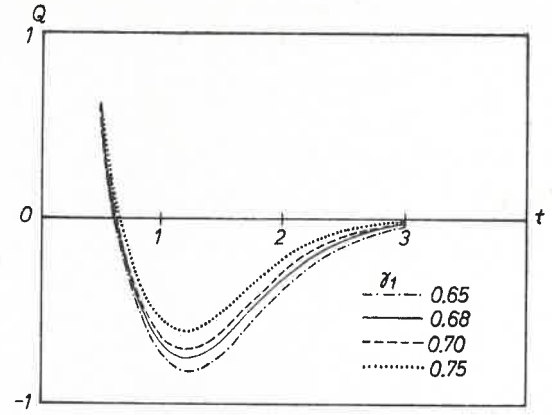

Fig. 4. The influence of parameter γ_1 on the quasi-potential

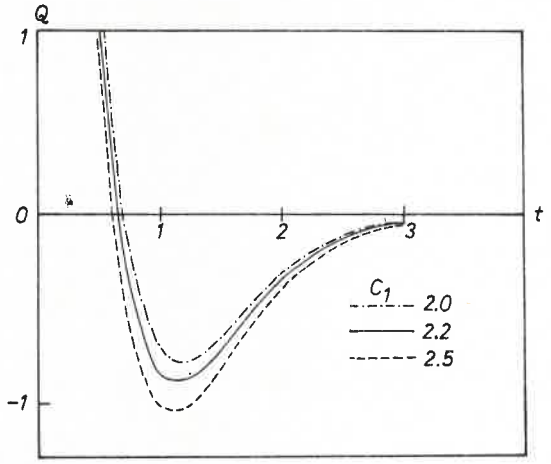

Fig. 5. The influence of parameter C_1 on the quasi-potential

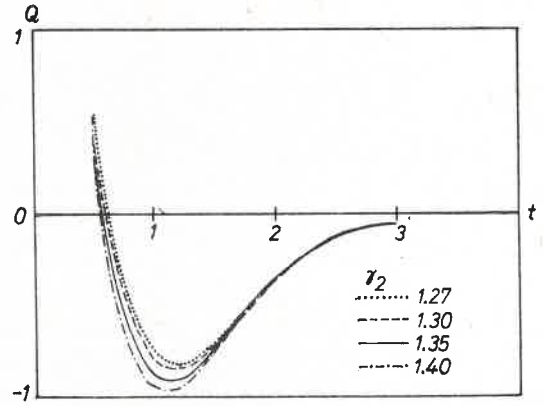

Fig. 6. The influence of parameter γ_2 on the quasi-potential

to adjust the width of the quasi-potential well and to modify the steepness of the repulsive slope at small values of t. Fig. 7 shows the quasi-potential for different energies. The behaviour shows that for increasing values of K, the quasipotential tends to be close to the

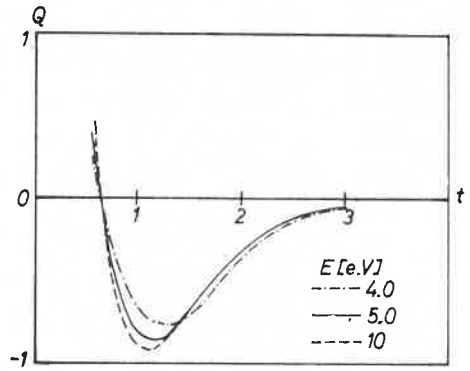

Fig. 7. The dependence of the quasi-potential on the energy E [e.V]

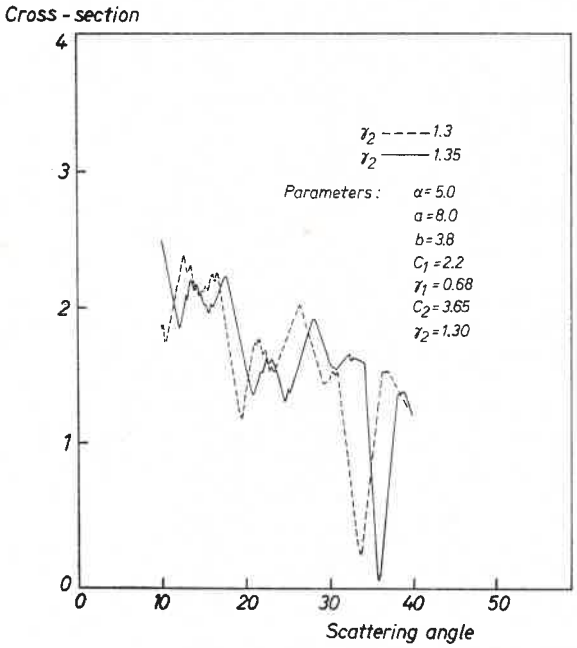

Fig. 8. Cross-section for two different values of the parameter γ_2

potential $P(x)$, which can be seen in Eq. (3). Fig. 8 gives the behavior of the cross--section for two different values of the parameter γ_2, which gives the deepness of the well.

Finally we find that for practical evaluations, the ten-parameter formulae (9) may be used to reproduce the experimental cross-section so that under the conditions described above the phase-function can be deduced.

Our program is now being used for the evaluation of scattering data obtained by our experimental groups in atom collisions. All the programs are written in PL/1. At present, we are extending this formalism to processes such as electronic transitions in ion-atom collisions which take place via a crossing of two potential curves.

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